ASCONA: Rapid Detection and Alignment of Protein Binding Site Conformations

Supporting Information

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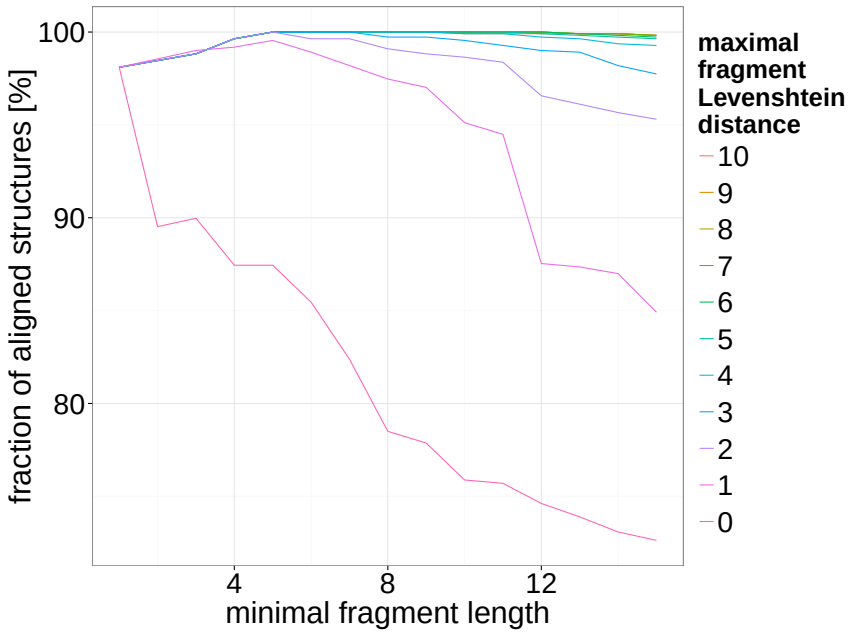

Figure S1: Fraction of successfully aligned Astex Non-Native structures as a function of l_f and k_f. Fixed parameter: $i_s = 1.0$. A subset of this data is depicted in Fig. 6.

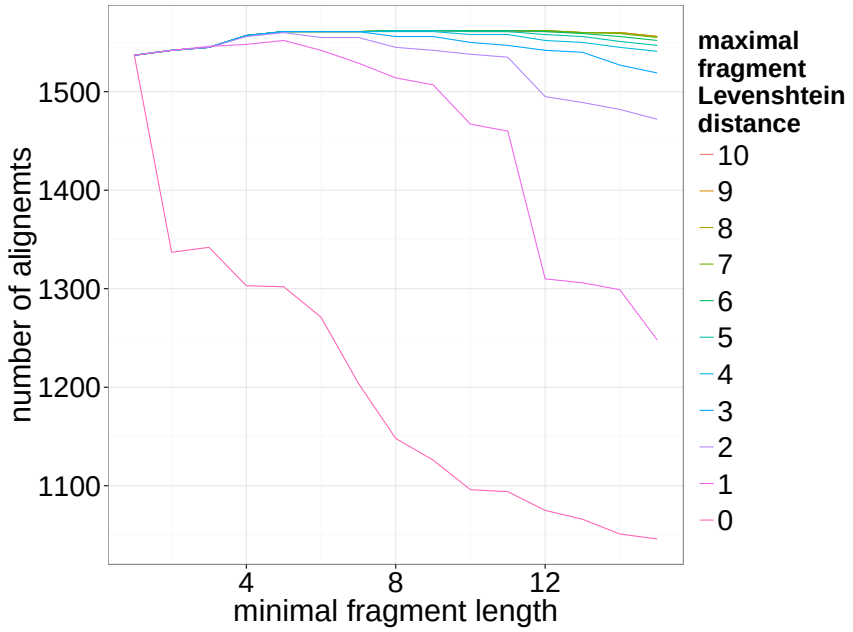

Figure S2: Total number of alignments for Astex Non-Native structures as a function of l_f and k_f. Fixed parameter: $i_s = 1.0$.

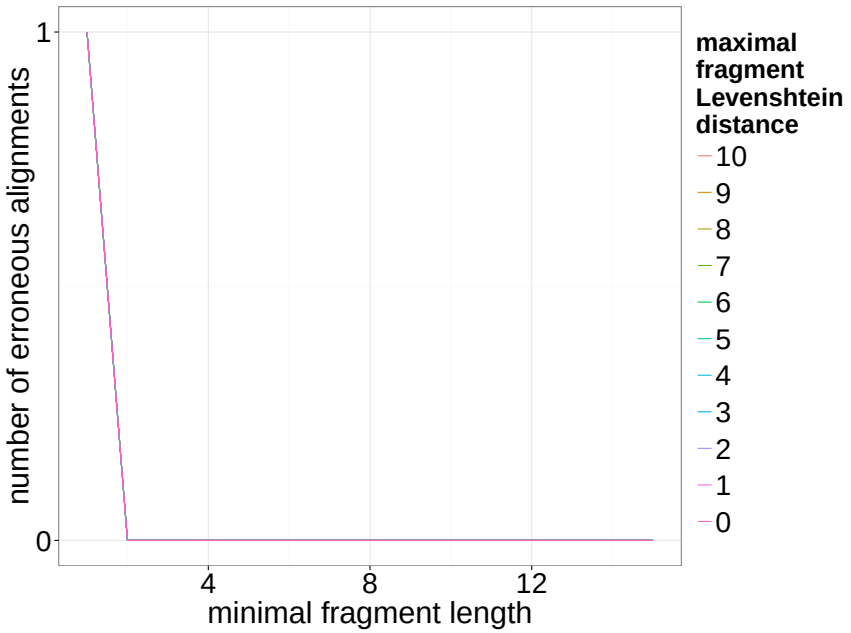

Figure S3: Total number of alignments resulting from Astex Non-Native structures that were mistakenly aligned against other reference active sites as a function of l_f and k_f. Fixed parameter: $i_s = 1.0$.

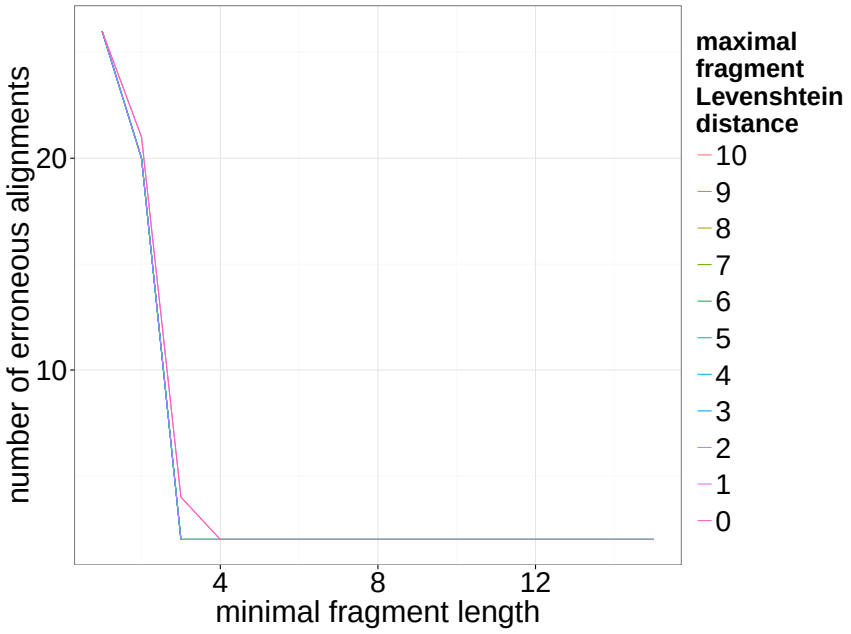

Figure S4: Total number of erroneous alignments for structures from the VPA set against l_f and k_f. Errors are detected by inconsistencies with the PDB annotation. Fixed parameter: $i_s = 1.0$.

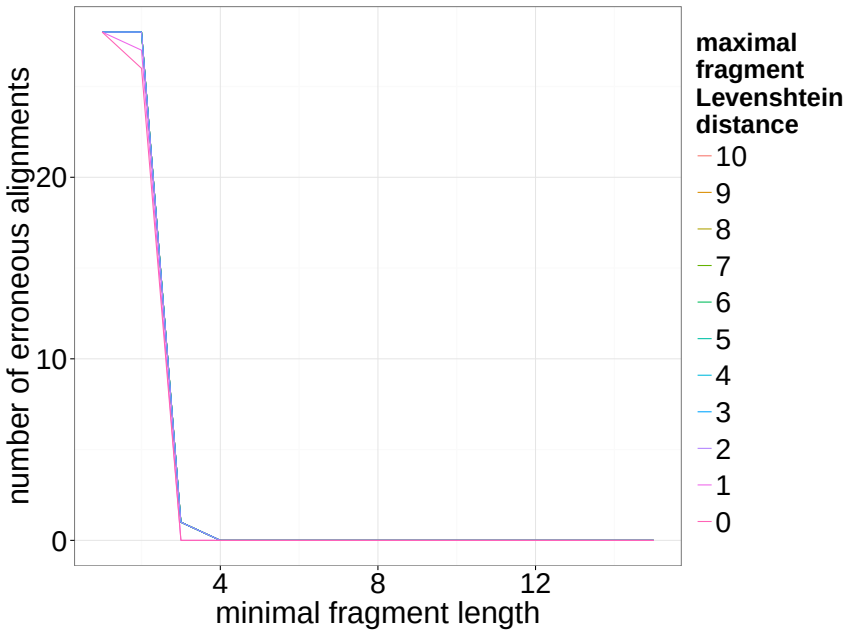

Figure S5: Total number of manually detected erroneous alignments from the Non-VPA set against l_f and k_f. Fixed parameter: $i_s = 1.0$.

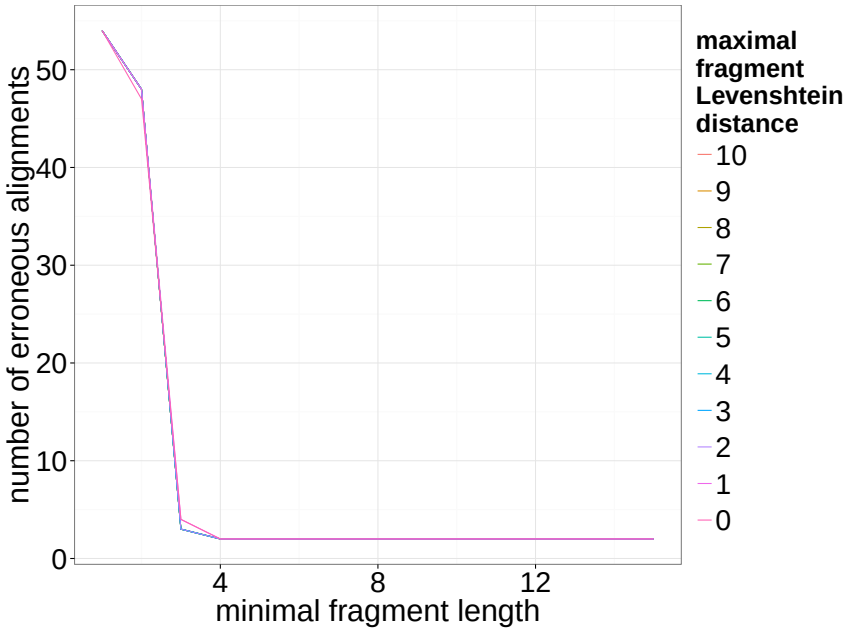

Figure S6: Total number of erroneous alignments for Astex Non-Native structures against l_f and k_f. Errors are detected by inconsistencies with the PDB annotation or manually inspection. Fixed parameter: $i_s = 1.0$.

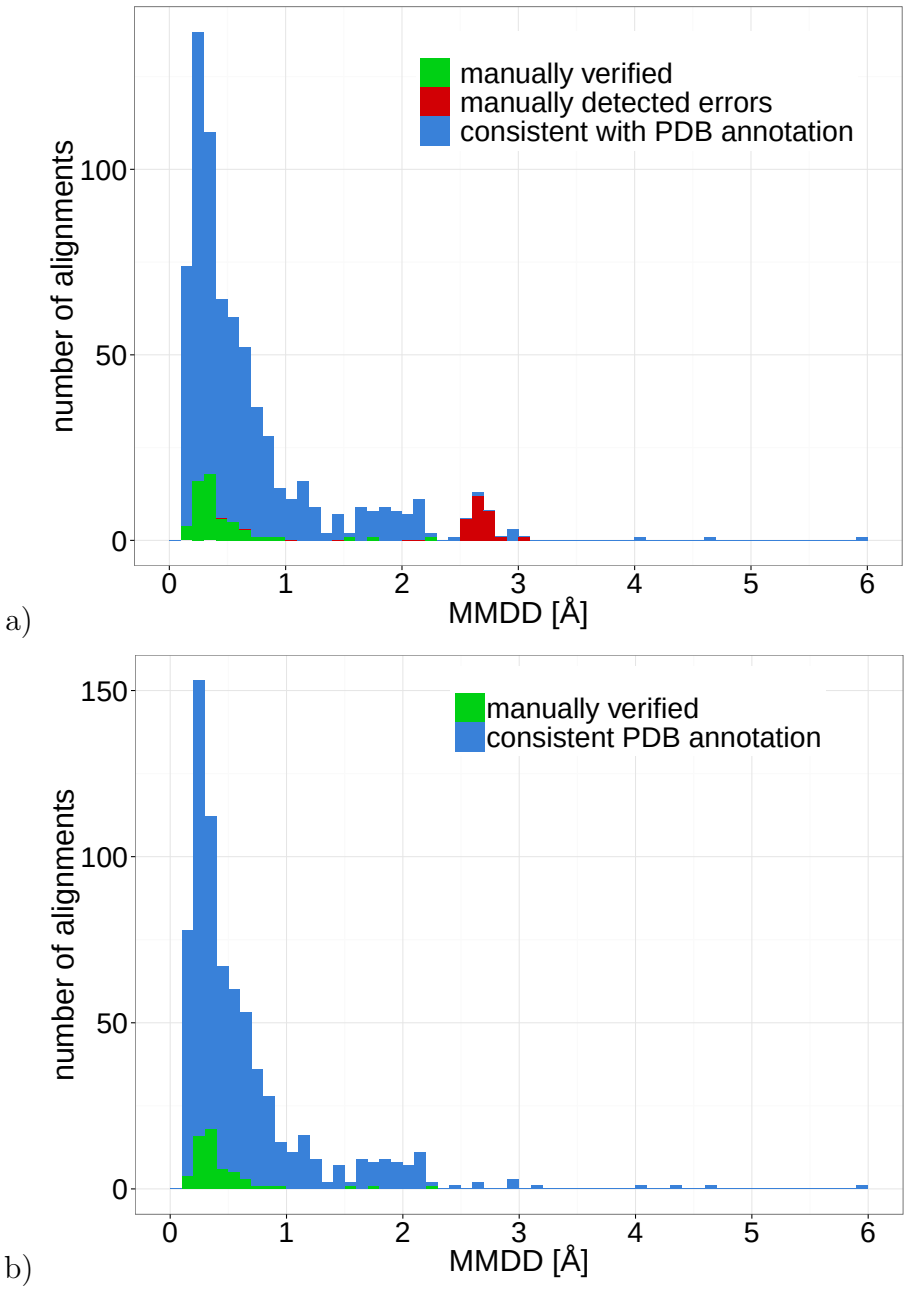

Figure S7: MMDD distribution over all alignments detected in the Non-VPA set. Applied parameters: a) $i_s = 1.0$, $l_f = 1$, $k_f = 1$; b) $i_s = 1.0$, $l_f = 7$, $k_f = 3$.

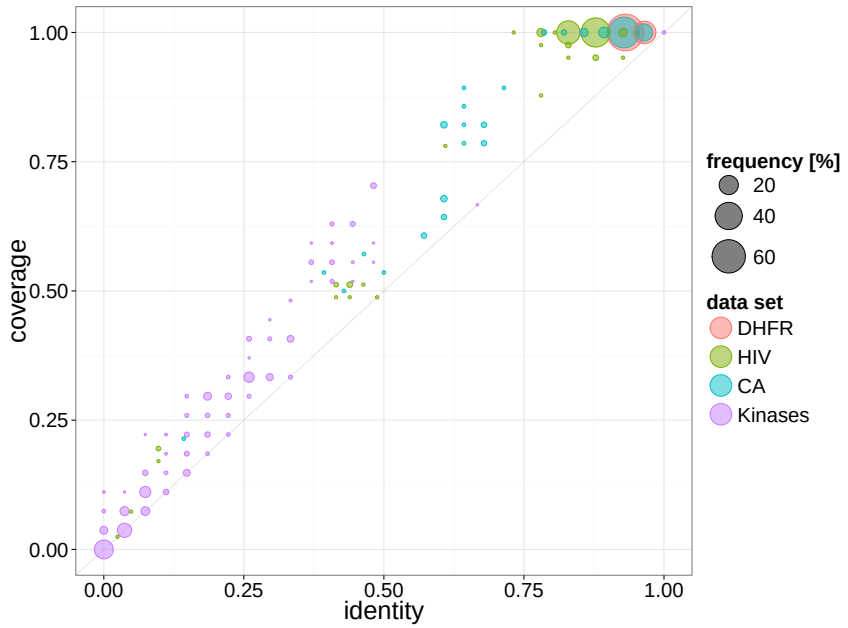

Figure S8: Alignment coverage against identity for all structures from four different mutation data sets. If more than one alignment was detected for a certain structure, only the one with the highest identity was used in the plot. Applied parameters: $i_s = 0.0$, $l_f = 7$, $k_f = 3$.

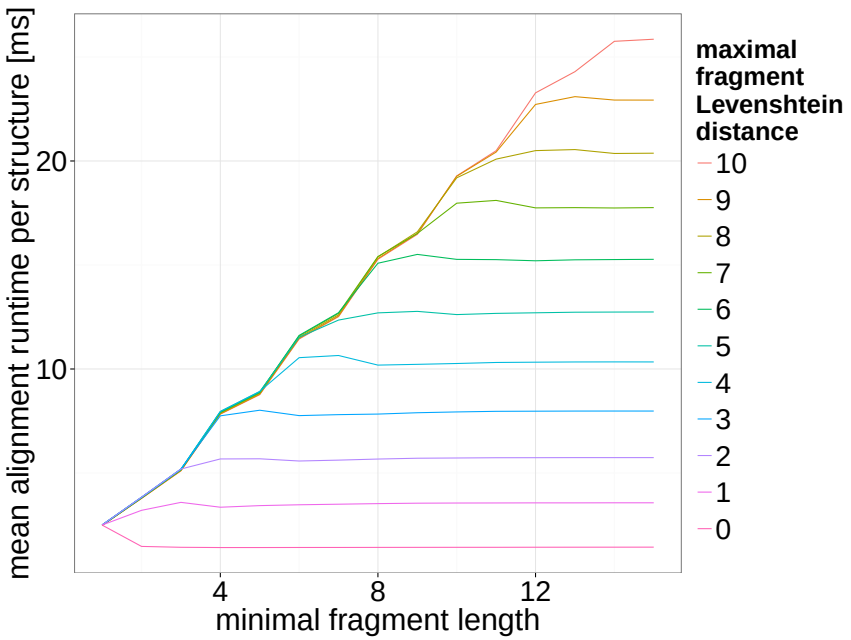

Figure S9: Average alignment runtime for an Astex Non-Native structure against a query binding site from another protein as a function of l_f and k_f. Fixed parameter: $i_s = 1.0$.

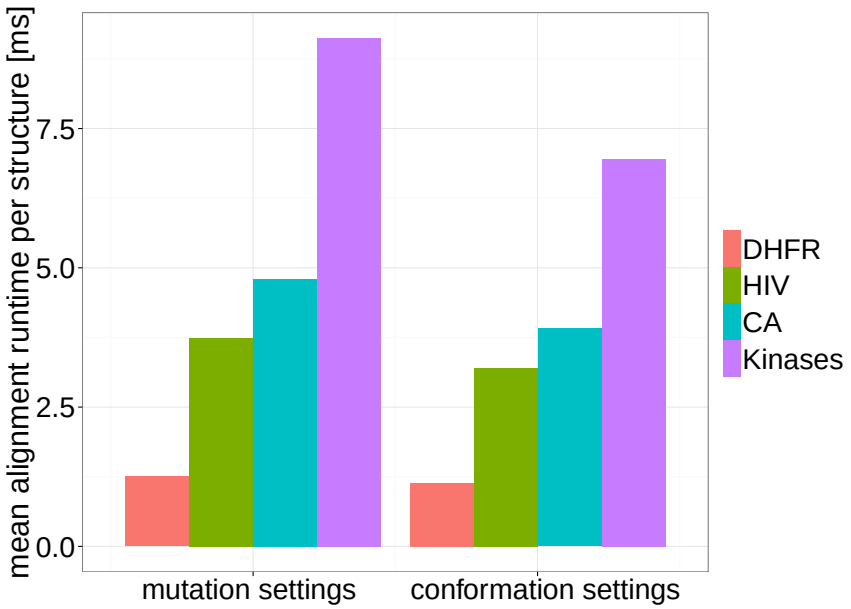

Figure S10: Average alignment runtime for a structure from the mutation data sets. Mutation settings: $i_s = 0.0$, $l_f = 10$, $k_f = 4$, conformation settings: $i_s = 0.0$, $l_f = 7$, $k_f = 3$

Table S1: PDB query details for the construction of the mutation data sets.

data set	EC number	taxonomy	sequence identity filter
DHFR	1.5.1.3	Homo sapiens	100%
HIV	3.4.23.16	Human immunodeficiency virus 1	100%
CA	4.2.1.1	Mammalia	100%
Kinases	2.7.10	Homo sapiens	100%

Table S2: Additional information on the mutation data sets.

data set	reference structure (PDB code)	reference ligand (PDB identifier)	mean number of residues per structure
DHFR	3F8Y	DH1	186
HIV	2P3D	3TL (alternate location A)	205
CA	3KNE	DAW	296
Kinases	3DKC	ATP	442

Table S3: PDB codes of all structures in the mutation data sets.

data set	ensemble structures (PDB) codes
DHFR	1DLR 1DLS 1HFP 1HFQ 1KMV 1U71 3EIG 3F8Y 3GHC 3GHV 3NXO 3OAF
HIV	1A94 1A9M 1AAQ 1AID 1AXA 1B6J 1BDL 1BDQ 1BDR 1BWB 1D4S 1FB7 1FF0 1G6L 1GNM 1GNN 1HEF 1HIV 1HVH 1HVS 1IZI 1K1U 1K2B 1K2C 1MER 1MET 1MRX 1MTB 1NH0 1ODX 1ODY 1PRO 1RL8 1SDU 1SGU 1SP5 1T3R 1T7I 1TCX 1TW7 1Z8C 1ZPK 2AVM 2AVS 2AVV 2AZ9 2AZB 2B7Z 2FDD 2FGU 2FGV 2FNS 2FNT 2FXD 2FXE 2G69 2HC0 2HS1 2HS2 2I4U 2I4V 2IAJ 2IAJ 2J9J 2J9J 2JE4 2JO0 2NMZ 2NNP 2NPH 2O40 2O4L 2O4N 2O4S 2P3A 2P3C 2P3D 2PYM 2PYN 2Q63 2Q64 2QCI 2QHC 2R38 2R43 2R8N 2RKF 2RKG 2WHH 2Z54 3A2O 3BVA 3BXR 3BXS 3CYW 3D1X 3D20 3D3T 3EKQ 3EKW 3EL4 3EL9 3EM3 3EM4 3FSM 3GGU 3HAU 3HAW 3HZC 3IA9 3IXO 3JVY 3JW2 3KA2 3KT2 3KT5 3LZS 3LZU 3LZV 3MWS 3N3I 3NWQ 3NXE 3O9I 3OQA 3OQD 3OU3 3OU4 3OU4 3OUB 3OUD 3OXV 3OXX 3OY4 3PJ6 3S43 3S54 3SPK 3T3C 3TTP 3U7S 3VF5 3VF7 3VFB 3ZPS 4DQB 4DQE 4DQF 4DQH 4EJ8 4EJD 4EPJ 4EQ0 4FLG 4FLG 4FLG 4GVM 4HEG 4ID1 4J55 4JMU 4K4R 4MC9 4OBF 4OBJ 4Q1W 4Q1X 4Q1Y 4QGI 4QJ6 4QJA 4QLH
CA	12CA 1BIC 1CAI 1CAJ 1CAM 1CAZ 1CCS 1CCT 1CCU 1CNG 1CNH 1CNI 1CNJ 1CNK 1CRM 1CVA 1CVD 1CVE 1CVF 1CVH 1DCB 1DMX 1FLJ 1FQL 1FR4 1FR7 1H9N 1H9Q 1HCB 1HEA 1HEB 1HEC 1HED 1I9Q 1JV0 1KEQ 1LG5 1LZV 1MOO 1MUA 1RJ6 1TG3 1TH9 1UGA 1UGB 1UGC 1UGD 1UGE 1UGF 1URT 1V9E 1V9I 1YDB 1YO1 1Z93 1Z97 1ZH9 1ZSC 2FNK 2FNN 2H4N 2HFW 2HKF 2NWO 2NWY 2NXT 2W2J 2ZNC 3DV7 3DVB 3DVC 3DVD 3FE4 3FW3 3IAI 3KNE 3KS3 3M1W 3MDZ 3ML5 3MNH 3MNI 3MNJ 3MNK 3OKV 3PJJ 3RG4 3RLD 3RYY 3TVN 3U45 3U47 3U7C 3UYN 3UYQ 3V3F 3V3G 3V3H 3V3I 3V3J 4CNR 4CNV 4CNW 4CNX 4GL1 4HBA 4HT2 4IDR 4JSA 4JSZ 4K13 4KNN 4L5U 4L5V 4L5W 4LU3 4M2V 4M2W 4Q07 4Q08 4QEF 4QK1 4QK2 4QK3 5CA2 6CA2 7CA2 8CA2 9CA2
Kinases	1A1A 1A81 1AB2 1AD5 1AOT 1AWO 1AWW 1B4F 1B55 1BTK 1BU1 1BWN 1BYG 1CF4 1CSK 1CSY 1EFN 1EV2 1EVT 1F62 1FBV 1FLT 1FMK 1FVR 1FYR 1G83 1GQ5 1H9O 1HCF 1HE7 1I44 1IGR 1II4 1IJR 1IR3 1K04 1K3A 1LCK 1LKK 1M6B 1MFG 1MFL 1MOX 1MQB 1MW4 1N8Z 1NQL 1NUN 1O4R 1OEC 1OPL 1P14 1P4O 1Q68 1QCF 1QLY 1QPC 1QPD 1QR1 1QU6 1RHF 1RJA 1RJB 1RY7 1SHC 1SHY 1SSL 1T46 1U59 1UCV 1WA7 1WWB 1WWC 1WWW 1X5L 1X6G 1X8B 1XR0 1YI6 1YOJ 1YOL 1YRK 1YVJ 1YY9 1Z9I 1ZZP 2A19 2A91 2ABL 2AHX 2B7A 2BBA 2BUJ 2C5D 2CBL 2CR3 2DBJ 2DCR 2DJS 2DM0 2DQ7 2DTG 2E6I 2E7H 2E8N 2E9W 2EAO 2EC8 2ECD 2EKX 2F4J 2FDB 2FO0 2GE9 2GY5 2H8H 2HDA 2HK5 2HR7 2HZI 2I1M 2IFG 2IIM 2ITN 2IVV 2K1L 2K9Y 2KGT 2KK1 2KK6 2KS1 2KSO 2KUP 2KUQ 2L4K 2L6W 2L9U 2LCT 2LCX 2LMJ 2LUL 2LZL 2M0B 2M20 2M59 2MC1 2MET 2MEU 2MFQ 2MFR 2OH4 2OJ2 2OQ1 2OZO 2PSQ 2PVF 2PVF 2PVY 2PWL 2PY3 2PZ5 2PZP 2PZR 2Q0B 2QBX 2QKQ 2QOD 2QOK 2QOL 2QON 2QOO 2R2P 2R4B 2REI 2RFE 2UZX 2VIF 2VWX 2W1I 2WO1 2WUH 2X1W 2X2U 2XA4 2XIR 2Y1N 2YHV 2YJR 2YJS 2YN8 2YS2 2YS5 2YUQ 2YUU 3A4O 3AOX 3B2T 3BEA 3BKB 3BRB 3BRH 3BU3 3BUO 3BUW 3BUX 3C1X 3C4F 3C7Q 3C8X 3CAF 3CC6 3CJF 3D7T 3D7T 3DKC 3DKG 3DPK 3EAC 3EAZ 3EFL 3EG0 3EG1 3EWH 3EYG 3F66 3FL7 3G0F 3G5V 3G5Y 3GEN 3GM3 3GOP 3GQI 3GRW 3H0F 3H0H 3H3B 3H8M 3HCK 3HEI 3HIL 3HMI 3HNG 3K2M 3K54 3KEX 3KKA 3KUL 3KVQ 3KXX 3L9P 3LCD 3LCO 3LMG 3LOH 3LXL 3LXP 3LZB 3MBW 3MJG 3MX0 3NHN 3NRU 3NW7 3NZ0 3OB2 3OCT 3OJ2 3OJM 3OJV 3OP0 3P0Y 3P11 3P1I 3PFV 3PJC 3PLS 3POZ 3PP0 3QGY 3QRJ 3QS7 3QS9 3QWQ 3RBB 3REA 3REB 3RI1 3S35 3SXS 3T9T 3TT0 3U2P 3U3F 3U6J 3UA7 3UGC 3UIU 3ULR 3US4 3V2A 3V5L 3V5Q 3V6B 3VHE 3VJN 3VO3 3VRO 3VRP 3VRR 3VW8 3W11 3W12 3W13 3W14 3W2P 3ZBF 3ZFM 3ZFX 3ZFY 3ZMP 3ZMQ 3ZNI 3ZON 4A4B 4A4C 4AG4 4ANL 4ANS 4ASE 4AT5 4AW5 4BBF 4BK5 4BKF 4BKJ 4BKY 4BSJ 4BSK 4C3F 4C61 4C8B 4CKI 4CKJ 4CLJ 4CRP 4D2W 4D8D 4D8K 4DKD 4DYL 4E6Q 4EIH 4EKU 4ET7 4F5B 4FL2 4FL3 4FNW 4FNX 4FOC 4FVQ 4FVR 4FWW 4FYO 4GFO 4GFU 4GIH 4GS0 4GT4 4GVJ 4HCK 4HCU 4HJO 4HRL 4HRN 4HVS 4HW7 4HXJ 4HZR 4HZS 4I20 4I22 4I24 4I4E 4I6Q 4IBM 4IVA 4IXP 4J96 4J97 4J98 4J99 4J9C 4J9E 4J9F 4K0V 4K11 4K2R 4K33 4K3J 4K94 4KRM 4KRP 4L00 4L01 4L0P 4L7S 4LEO 4LIQ 4LQM 4LRM 4M4P 4MXX 4MXY 4NY0 4O3U 4OGA 4OGA 4OLI 4ORZ 4OTW 4P2K 4PMP 4PO6 4PQN 4PX6 4PY1 4QPS 4QQ5 4QQC 4QQJ 4QQT 4QT8 4R32 4RA0 4RFZ 4RIX 4RIY 4RIY 4RJ8 4TYG 4U5W 4UMQ 4UMT 4UX0 4UX8 4UXQ 4W50 4WUN 4X3J

Table S4: Background information for cases from the CA and HIV mutation data sets with a coverage below 1.0

data set	case description	PDB codes
CA	different protein (carbonic anhydrase I)	1CRM 1HCB 1JV0
CA	different protein (carbonic anhydrase III)	2HFW 1FLJ 1Z97 1Z93 3UYN 3UYQ
CA	different protein (carbonic anhydrase IV)	2ZNC 3FW3
CA	different protein (carbonic anhydrase V)	1KEQ 1URT 1DMX
CA	different protein (carbonic anhydrase VI)	3FE4
CA	different protein (carbonic anhydrase VII)	3MDZ 3ML5
CA	different protein (carbonic anhydrase VIII)	2W2J
CA	different protein (carbonic anhydrase IX)	3IAI
CA	different protein (carbonic anhydrase XII)	4HT2
CA	different protein (carbonic anhydrase XIII)	4KNN
CA	different protein (carbonic anhydrase XIV)	1RJ6 4LU3
CA	different protein (antibody fragment Fab M75 complexed to short fragment of carbonic anhydrase IX)	2HKF
HIV	wrong EC annotation (HIV integrase)	4ID1 4GVM
HIV	wrong EC annotation (HIV reverse transcriptase)	2IAJ
HIV	wrong EC annotation (HIV matrix protein)	4JMU
HIV	wrong EC annotation (HIV capsid protein)	2JO0
HIV	one subunit only	1FB7 2G69 2AZB 3OQD 3OQA 3PJ6 2R8N 1HEF 2AZ9
HIV	non-amino acid residue (OIL) that cannot be aligned	3NWQ
HIV	missing fragment match due to early abort criterion	4EQ0 3NXE

Table S5: Coverage and identity values for all structures from the DHFR mutation data set. If more than one alignment was detected for a certain structure, only the one with the highest identity was selected.

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
1KMV	1.00	0.97	1.00	0.97
3GHV	1.00	0.97	1.00	0.97
3NXO	1.00	0.97	1.00	0.97
1DLR	1.00	0.93	1.00	0.93
1DLS	1.00	0.93	1.00	0.93
1HFP	1.00	0.93	1.00	0.93
1HFQ	1.00	0.93	1.00	0.93
1U71	1.00	0.93	1.00	0.93
3EIG	1.00	0.93	1.00	0.93
3GHC	1.00	0.93	1.00	0.93
3OAF	1.00	0.93	1.00	0.93

Table S6: Coverage and identity values for all structures from the HIV mutation data set. If more than one alignment was detected for a certain structure, only the one with the highest identity was selected.

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
2HC0	1.00	0.95	1.00	0.95
1HVS	1.00	0.93	1.00	0.93
1ODX	1.00	0.93	1.00	0.93
1RL8	1.00	0.93	1.00	0.93
2FDD	1.00	0.93	1.00	0.93
2NMZ	1.00	0.93	1.00	0.93
2P3A	1.00	0.93	0.95	0.93
2B7Z	1.00	0.88	1.00	0.93
2FXD	1.00	0.88	1.00	0.93
1A94	1.00	0.88	1.00	0.88
1AAQ	1.00	0.88	1.00	0.88

Continuation of Table S6

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
1AID	1.00	0.88	1.00	0.88
1B6J	1.00	0.88	1.00	0.88
1G6L	1.00	0.88	1.00	0.88
1GNM	1.00	0.88	1.00	0.88
1GNN	1.00	0.88	1.00	0.88
1HIV	1.00	0.88	1.00	0.88
1HVH	1.00	0.88	1.00	0.88
1K2B	1.00	0.88	1.00	0.88
1MET	1.00	0.88	1.00	0.88
1NH0	1.00	0.88	1.00	0.88
1ODY	1.00	0.88	1.00	0.88
1PRO	1.00	0.88	1.00	0.88
1SDU	1.00	0.88	1.00	0.88
1SP5	1.00	0.88	1.00	0.88
1T3R	1.00	0.88	1.00	0.88
2AVM	1.00	0.88	1.00	0.88
2AVV	1.00	0.88	1.00	0.88
2FNT	1.00	0.88	1.00	0.88
2FXE	1.00	0.88	1.00	0.88
2HS2	1.00	0.88	1.00	0.88
2I4U	1.00	0.88	1.00	0.88
2J9J	1.00	0.88	1.00	0.88
2JE4	1.00	0.88	1.00	0.88
2NPH	1.00	0.88	1.00	0.88
2O40	1.00	0.88	1.00	0.88
2O4S	1.00	0.88	1.00	0.88
2P3C	1.00	0.88	1.00	0.88
2WHH	1.00	0.88	1.00	0.88
3A2O	1.00	0.88	1.00	0.88
3BXS	1.00	0.88	1.00	0.88
3D1X	1.00	0.88	1.00	0.88
3D20	1.00	0.88	1.00	0.88
3EKW	1.00	0.88	1.00	0.88
3FSM	1.00	0.88	1.00	0.88
3HAU	1.00	0.88	1.00	0.88
3HAW	1.00	0.88	1.00	0.88
3HZC	1.00	0.88	1.00	0.88

Continuation of Table S6

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
3JVY	1.00	0.88	1.00	0.88
3JW2	1.00	0.88	1.00	0.88
3KA2	1.00	0.88	1.00	0.88
3KT2	1.00	0.88	1.00	0.88
3KT5	1.00	0.88	1.00	0.88
3LZS	1.00	0.88	1.00	0.88
3LZU	1.00	0.88	1.00	0.88
3MWS	1.00	0.88	1.00	0.88
3O9I	1.00	0.88	1.00	0.88
3VFB	1.00	0.88	1.00	0.88
4DQB	1.00	0.88	1.00	0.88
4DQE	1.00	0.88	1.00	0.88
4DQF	1.00	0.88	1.00	0.88
4DQH	1.00	0.88	1.00	0.88
4EJ8	1.00	0.88	1.00	0.88
4EJD	1.00	0.88	1.00	0.88
4K4R	1.00	0.88	1.00	0.88
4MC9	1.00	0.88	1.00	0.88
4Q1W	1.00	0.88	1.00	0.88
4QLH	1.00	0.88	1.00	0.88
1FF0	1.00	0.88	0.95	0.88
1K1U	1.00	0.88	0.95	0.88
1BDL	1.00	0.85	0.98	0.83
1BDR	1.00	0.85	0.98	0.83
1BWB	1.00	0.83	1.00	0.88
1D4S	1.00	0.83	1.00	0.88
1IZI	1.00	0.83	1.00	0.88
1MER	1.00	0.83	1.00	0.88
1MRX	1.00	0.83	1.00	0.88
1SGU	1.00	0.83	1.00	0.88
1T7I	1.00	0.83	1.00	0.88
1TW7	1.00	0.83	1.00	0.88
1Z8C	1.00	0.83	1.00	0.88
1ZPK	1.00	0.83	1.00	0.88
2I4V	1.00	0.83	1.00	0.88
2NNP	1.00	0.83	1.00	0.88
2R38	1.00	0.83	1.00	0.88

Continuation of Table S6

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
3EL4	1.00	0.83	1.00	0.88
3EL9	1.00	0.83	1.00	0.88
3T3C	1.00	0.83	1.00	0.88
3ZPS	1.00	0.83	1.00	0.88
1A9M	1.00	0.83	1.00	0.83
1AXA	1.00	0.83	1.00	0.83
1K2C	1.00	0.83	1.00	0.83
1MTB	1.00	0.83	1.00	0.83
2AVS	1.00	0.83	1.00	0.83
2FGU	1.00	0.83	1.00	0.83
2FGV	1.00	0.83	1.00	0.83
2FNS	1.00	0.83	1.00	0.83
2HS1	1.00	0.83	1.00	0.83
2O4L	1.00	0.83	1.00	0.83
2PYM	1.00	0.83	1.00	0.83
2PYN	1.00	0.83	1.00	0.83
2Q63	1.00	0.83	1.00	0.83
2Q64	1.00	0.83	1.00	0.83
2QCI	1.00	0.83	1.00	0.83
2QHC	1.00	0.83	1.00	0.83
2R43	1.00	0.83	1.00	0.83
2RKF	1.00	0.83	1.00	0.83
2RKG	1.00	0.83	1.00	0.83
2Z54	1.00	0.83	1.00	0.83
3BVA	1.00	0.83	1.00	0.83
3BXR	1.00	0.83	1.00	0.83
3CYW	1.00	0.83	1.00	0.83
3D3T	1.00	0.83	1.00	0.83
3EKQ	1.00	0.83	1.00	0.83
3EM3	1.00	0.83	1.00	0.83
3EM4	1.00	0.83	1.00	0.83
3IA9	1.00	0.83	1.00	0.83
3IXO	1.00	0.83	1.00	0.83
3LZV	1.00	0.83	1.00	0.83
3N3I	1.00	0.83	1.00	0.83
3OXV	1.00	0.83	1.00	0.83
3OXX	1.00	0.83	1.00	0.83

Continuation of Table S6

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
3OY4	1.00	0.83	1.00	0.83
3VF5	1.00	0.83	1.00	0.83
3VF7	1.00	0.83	1.00	0.83
4EPJ	1.00	0.83	1.00	0.83
4FLG	1.00	0.83	1.00	0.83
4HEG	1.00	0.83	1.00	0.83
4OBJ	1.00	0.83	1.00	0.83
4Q1X	1.00	0.83	1.00	0.83
4Q1Y	1.00	0.83	1.00	0.83
4QGI	1.00	0.83	1.00	0.83
4QJA	1.00	0.83	1.00	0.83
3GGU	1.00	0.83	0.95	0.88
1BDQ	1.00	0.80	0.98	0.78
3OU3	1.00	0.78	1.00	0.83
3OU4	1.00	0.78	1.00	0.83
3OUB	1.00	0.78	1.00	0.83
3SPK	1.00	0.78	1.00	0.83
3U7S	1.00	0.78	1.00	0.83
1TCX	1.00	0.78	1.00	0.78
3S43	1.00	0.78	1.00	0.78
3S54	1.00	0.78	1.00	0.78
3TTP	1.00	0.78	1.00	0.78
4OBF	1.00	0.78	1.00	0.78
4QJ6	1.00	0.78	1.00	0.78
2O4N	1.00	0.78	0.95	0.83
3OUD	1.00	0.76	1.00	0.80
4J55	1.00	0.68	1.00	0.73
3NWQ	0.95	0.83	0.98	0.83
3NXE	0.88	0.78	0.88	0.78
4EQ0	0.76	0.59	0.78	0.61
2AZ9	0.51	0.46	0.51	0.46
1HEF	0.51	0.44	0.51	0.44
2R8N	0.51	0.44	0.51	0.44
3PJ6	0.51	0.41	0.51	0.44
2G69	0.51	0.41	0.49	0.44
1FB7	0.51	0.41	0.49	0.41
3OQA	0.51	0.39	0.51	0.41

Continuation of Table S6

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
3OQD	0.51	0.39	0.51	0.41
2AZB	0.49	0.46	0.49	0.49
4GVM	-	-	0.20	0.10
4ID1	-	-	0.20	0.10
2IAJ	-	-	0.17	0.10
4JMU	-	-	0.07	0.05
2JO0	-	-	0.02	0.02

Table S7: Coverage and identity values for all structures from the CA mutation data set. If more than one alignment was detected for a certain structure, only the one with the highest identity was selected.

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
1CNG	1.00	0.96	1.00	0.96
1MOO	1.00	0.96	1.00	0.96
1ZH9	1.00	0.96	1.00	0.96
1ZSC	1.00	0.96	1.00	0.96
2FNK	1.00	0.96	1.00	0.96
3KS3	1.00	0.96	1.00	0.96
3M1W	1.00	0.96	1.00	0.96
3MNH	1.00	0.96	1.00	0.96
3MNI	1.00	0.96	1.00	0.96
3MNJ	1.00	0.96	1.00	0.96
3MNK	1.00	0.96	1.00	0.96
3PJJ	1.00	0.96	1.00	0.96
3RYY	1.00	0.96	1.00	0.96
3V3F	1.00	0.96	1.00	0.96
4HBA	1.00	0.96	1.00	0.96
4L5U	1.00	0.96	1.00	0.96
4L5V	1.00	0.96	1.00	0.96
4L5W	1.00	0.96	1.00	0.96
4QK1	1.00	0.96	1.00	0.96

Continuation of Table S7

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
4QK2	1.00	0.96	1.00	0.96
4QK3	1.00	0.96	1.00	0.96
12CA	1.00	0.93	1.00	0.93
1BIC	1.00	0.93	1.00	0.93
1CAI	1.00	0.93	1.00	0.93
1CAJ	1.00	0.93	1.00	0.93
1CAM	1.00	0.93	1.00	0.93
1CAZ	1.00	0.93	1.00	0.93
1CCS	1.00	0.93	1.00	0.93
1CCT	1.00	0.93	1.00	0.93
1CCU	1.00	0.93	1.00	0.93
1CNH	1.00	0.93	1.00	0.93
1CNI	1.00	0.93	1.00	0.93
1CNJ	1.00	0.93	1.00	0.93
1CNK	1.00	0.93	1.00	0.93
1CVA	1.00	0.93	1.00	0.93
1CVD	1.00	0.93	1.00	0.93
1CVE	1.00	0.93	1.00	0.93
1CVF	1.00	0.93	1.00	0.93
1CVH	1.00	0.93	1.00	0.93
1DCB	1.00	0.93	1.00	0.93
1FQL	1.00	0.93	1.00	0.93
1FR4	1.00	0.93	1.00	0.93
1FR7	1.00	0.93	1.00	0.93
1H9N	1.00	0.93	1.00	0.93
1H9Q	1.00	0.93	1.00	0.93
1HEA	1.00	0.93	1.00	0.93
1HEB	1.00	0.93	1.00	0.93
1HEC	1.00	0.93	1.00	0.93
1HED	1.00	0.93	1.00	0.93
1I9Q	1.00	0.93	1.00	0.93
1LG5	1.00	0.93	1.00	0.93
1LZV	1.00	0.93	1.00	0.93
1MUA	1.00	0.93	1.00	0.93
1TG3	1.00	0.93	1.00	0.93
1TH9	1.00	0.93	1.00	0.93
1UGA	1.00	0.93	1.00	0.93

Continuation of Table S7

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
1UGB	1.00	0.93	1.00	0.93
1UGC	1.00	0.93	1.00	0.93
1UGD	1.00	0.93	1.00	0.93
1UGE	1.00	0.93	1.00	0.93
1UGF	1.00	0.93	1.00	0.93
1YDB	1.00	0.93	1.00	0.93
1YO1	1.00	0.93	1.00	0.93
2FNN	1.00	0.93	1.00	0.93
2H4N	1.00	0.93	1.00	0.93
2NWO	1.00	0.93	1.00	0.93
2NWY	1.00	0.93	1.00	0.93
2NXT	1.00	0.93	1.00	0.93
3DV7	1.00	0.93	1.00	0.93
3DVB	1.00	0.93	1.00	0.93
3DVC	1.00	0.93	1.00	0.93
3DVD	1.00	0.93	1.00	0.93
3RG4	1.00	0.93	1.00	0.93
3RLD	1.00	0.93	1.00	0.93
3TVN	1.00	0.93	1.00	0.93
3U45	1.00	0.93	1.00	0.93
3U47	1.00	0.93	1.00	0.93
3U7C	1.00	0.93	1.00	0.93
3V3G	1.00	0.93	1.00	0.93
4JSA	1.00	0.93	1.00	0.93
4JSZ	1.00	0.93	1.00	0.93
4QEF	1.00	0.93	1.00	0.93
5CA2	1.00	0.93	1.00	0.93
6CA2	1.00	0.93	1.00	0.93
7CA2	1.00	0.93	1.00	0.93
8CA2	1.00	0.93	1.00	0.93
9CA2	1.00	0.93	1.00	0.93
1V9E	1.00	0.89	1.00	0.89
1V9I	1.00	0.89	1.00	0.89
3OKV	1.00	0.89	1.00	0.89
3V3H	1.00	0.89	1.00	0.89
3V3I	1.00	0.89	1.00	0.89
4CNV	1.00	0.89	1.00	0.89

Continuation of Table S7

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
4GL1	1.00	0.89	1.00	0.89
4IDR	1.00	0.89	1.00	0.89
3V3J	1.00	0.86	1.00	0.86
4CNR	1.00	0.86	1.00	0.86
4CNW	1.00	0.86	1.00	0.86
4CNX	1.00	0.86	1.00	0.86
4K13	1.00	0.86	1.00	0.86
4M2V	1.00	0.82	1.00	0.82
4M2W	1.00	0.82	1.00	0.82
4Q07	1.00	0.79	1.00	0.79
4Q08	1.00	0.79	1.00	0.79
2HFW	0.89	0.64	0.86	0.64
4KNN	0.86	0.68	0.89	0.71
1FLJ	0.86	0.64	0.89	0.64
1KEQ	0.79	0.64	0.82	0.68
1URT	0.79	0.64	0.82	0.68
1DMX	0.79	0.61	0.79	0.64
1Z97	0.75	0.61	0.82	0.64
1Z93	0.75	0.57	0.82	0.61
3UYN	0.75	0.57	0.82	0.61
3UYQ	0.75	0.57	0.82	0.61
3MDZ	0.71	0.68	0.79	0.68
3ML5	0.71	0.68	0.79	0.68
1CRM	0.71	0.61	0.68	0.61
1HCB	0.71	0.61	0.68	0.61
1JV0	0.71	0.61	0.68	0.61
3FE4	0.43	0.39	0.64	0.61
1RJ6	0.39	0.36	0.64	0.61
2W2J	0.39	0.29	0.54	0.39
4LU3	0.36	0.32	0.61	0.57
4HT2	0.36	0.32	0.54	0.50
3IAI	0.32	0.29	0.61	0.57
3FW3	0.25	0.18	0.57	0.46
2ZNC	0.25	0.18	0.50	0.43
2HKF	-	-	0.21	0.14

Table S8: Coverage and identity values for all structures from the Kinase mutation data set. If more than one alignment was detected for a certain structure, only the one with the highest identity was selected.

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
3C1X	1.00	1.00	1.00	1.00
3F66	1.00	1.00	1.00	1.00
3VW8	1.00	1.00	1.00	1.00
3PLS	1.00	0.85	1.00	0.85
3DKG	0.67	0.67	0.67	0.67
3PP0	0.63	0.37	0.33	0.22
2R4B	0.59	0.37	0.33	0.26
3W2P	0.59	0.37	0.30	0.19
4HJO	0.59	0.37	0.30	0.19
4I20	0.59	0.37	0.30	0.19
4I24	0.59	0.37	0.30	0.19
4LQM	0.59	0.37	0.30	0.19
4LRM	0.59	0.37	0.30	0.19
4RIX	0.59	0.37	0.30	0.19
4RIY	0.59	0.37	0.30	0.19
1FVR	0.56	0.41	0.63	0.44
2REI	0.56	0.37	0.59	0.37
1MQB	0.56	0.37	0.56	0.37
2R2P	0.56	0.37	0.56	0.37
2VWX	0.56	0.37	0.56	0.37
4P2K	0.56	0.37	0.56	0.37
2RFE	0.56	0.33	0.30	0.19
3LZB	0.56	0.33	0.30	0.19
3POZ	0.56	0.33	0.30	0.19
4I22	0.56	0.33	0.26	0.15
4RJ8	0.56	0.33	0.26	0.15
3BRB	0.52	0.44	0.59	0.48
1IR3	0.52	0.33	0.52	0.41
3BU3	0.52	0.33	0.52	0.41
4IBM	0.52	0.33	0.52	0.41

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
4AW5	0.48	0.33	0.56	0.37
2YN8	0.48	0.33	0.48	0.33
1T46	0.48	0.33	0.41	0.33
2I1M	0.48	0.33	0.41	0.33
3BEA	0.48	0.33	0.41	0.33
3DPK	0.48	0.33	0.41	0.33
3G0F	0.48	0.33	0.41	0.33
3LCO	0.48	0.33	0.41	0.33
4HVS	0.48	0.33	0.41	0.33
4HW7	0.48	0.33	0.41	0.33
3LCD	0.48	0.33	0.33	0.30
3ZFX	0.48	0.33	0.26	0.19
1I44	0.48	0.30	0.52	0.41
1P14	0.48	0.26	0.48	0.33
3BKB	0.44	0.37	0.56	0.48
4BKJ	0.41	0.37	0.52	0.44
3V5Q	0.41	0.33	0.56	0.44
4AT5	0.41	0.33	0.56	0.44
4PMP	0.41	0.30	0.56	0.41
2IVV	0.41	0.26	0.41	0.26
4CKJ	0.41	0.26	0.41	0.26
4GT4	0.41	0.22	0.41	0.26
4CKI	0.37	0.22	0.41	0.26
4ANL	0.26	0.22	0.41	0.33
4ANS	0.26	0.22	0.41	0.33
4K33	0.26	0.22	0.41	0.30
4QQJ	0.26	0.22	0.41	0.30
4QQT	0.26	0.22	0.41	0.30
4TYG	0.26	0.22	0.41	0.30
1OEC	0.26	0.22	0.33	0.30
2PVF	0.26	0.22	0.33	0.30
3C4F	0.26	0.22	0.33	0.30
3GQI	0.26	0.22	0.33	0.30
3TT0	0.26	0.22	0.33	0.30
4J97	0.26	0.22	0.33	0.30
4UX0	0.26	0.22	0.33	0.30
4WUN	0.26	0.22	0.33	0.30

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
2PSQ	0.26	0.22	0.33	0.26
2PVY	0.26	0.22	0.33	0.26
2PWL	0.26	0.22	0.33	0.26
2PY3	0.26	0.22	0.33	0.26
2PZ5	0.26	0.22	0.33	0.26
2PZP	0.26	0.22	0.33	0.26
2PZR	0.26	0.22	0.33	0.26
2Q0B	0.26	0.22	0.33	0.26
3B2T	0.26	0.22	0.33	0.26
3KXX	0.26	0.22	0.33	0.26
3RI1	0.26	0.22	0.33	0.26
4J96	0.26	0.22	0.33	0.26
4J98	0.26	0.22	0.33	0.26
4J99	0.26	0.22	0.33	0.26
4QQC	0.26	0.22	0.33	0.22
4QQ5	0.26	0.22	0.19	0.19
4UXQ	0.26	0.22	0.19	0.19
2OH4	0.26	0.19	0.70	0.48
2XIR	0.26	0.19	0.70	0.48
3HNG	0.26	0.19	0.70	0.48
3U6J	0.26	0.19	0.70	0.48
3VHE	0.26	0.19	0.70	0.48
3VO3	0.26	0.19	0.70	0.48
4ASE	0.26	0.19	0.70	0.48
1RJB	0.26	0.19	0.41	0.33
3VJN	0.26	0.19	0.30	0.19
3SXS	0.26	0.19	0.22	0.19
2F4J	0.22	0.22	0.33	0.33
2HZI	0.22	0.22	0.33	0.33
3HMI	0.22	0.22	0.33	0.33
3QRJ	0.22	0.22	0.33	0.33
1OPL	0.22	0.19	0.33	0.30
2FO0	0.22	0.19	0.33	0.30
1YVJ	0.22	0.19	0.30	0.26
3LXL	0.22	0.19	0.30	0.26
3PJC	0.22	0.19	0.30	0.26
4I6Q	0.22	0.19	0.30	0.26

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
1K3A	0.22	0.19	0.26	0.22
3NW7	0.22	0.19	0.26	0.22
1P4O	0.22	0.19	0.19	0.19
1YI6	0.22	0.19	0.15	0.15
2H8H	0.22	0.19	0.15	0.15
4K11	0.22	0.19	0.15	0.15
3EWH	0.22	0.15	0.70	0.48
3EYG	0.22	0.15	0.63	0.44
3LXP	0.22	0.15	0.63	0.44
4GVJ	0.22	0.15	0.63	0.44
4PY1	0.22	0.15	0.63	0.44
1BYG	0.22	0.15	0.59	0.41
4HZR	0.22	0.15	0.33	0.22
2B7A	0.22	0.15	0.30	0.22
2W1I	0.22	0.15	0.30	0.22
2XA4	0.22	0.15	0.30	0.22
3UGC	0.22	0.15	0.30	0.22
4C61	0.22	0.15	0.30	0.22
4E6Q	0.22	0.15	0.30	0.22
4HZS	0.22	0.15	0.30	0.22
4IVA	0.22	0.15	0.30	0.22
4QPS	0.22	0.15	0.30	0.22
4OTW	0.22	0.15	0.26	0.19
2ITN	0.22	0.15	0.26	0.15
2QOK	0.22	0.15	0.22	0.15
2QON	0.22	0.15	0.22	0.15
3KEX	0.22	0.15	0.22	0.15
3KUL	0.22	0.15	0.22	0.15
3LMG	0.22	0.15	0.22	0.15
3NZ0	0.22	0.11	0.63	0.41
4GFO	0.22	0.11	0.63	0.41
4GIH	0.22	0.11	0.63	0.41
4OLI	0.22	0.11	0.63	0.41
3C7Q	0.19	0.15	0.63	0.44
3D7T	0.19	0.15	0.41	0.26
3ZBF	0.19	0.15	0.33	0.30
2YHV	0.19	0.15	0.33	0.26

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
2YJR	0.19	0.15	0.33	0.26
2YJS	0.19	0.15	0.33	0.26
3AOX	0.19	0.15	0.33	0.26
3L9P	0.19	0.15	0.33	0.26
4CLJ	0.19	0.15	0.33	0.26
4FL2	0.19	0.15	0.33	0.26
4FNW	0.19	0.15	0.33	0.26
4FNX	0.19	0.15	0.33	0.26
4FOC	0.19	0.15	0.33	0.26
3CC6	0.19	0.15	0.22	0.19
3GEN	0.19	0.15	0.22	0.19
4RFZ	0.19	0.15	0.22	0.19
1FMK	0.19	0.15	0.22	0.07
3K54	0.19	0.15	0.19	0.15
3OCT	0.19	0.15	0.19	0.15
4MXY	0.19	0.15	0.11	0.11
4MXX	0.19	0.11	0.11	0.07
3T9T	0.15	0.15	0.56	0.41
4HCU	0.15	0.15	0.56	0.41
3CJF	0.15	0.11	0.59	0.41
4I4E	0.15	0.11	0.52	0.37
3EFL	0.15	0.11	0.37	0.26
4FL3	0.15	0.11	0.33	0.26
3ZFY	0.15	0.11	0.30	0.22
4FYO	0.15	0.11	0.26	0.22
4PX6	0.15	0.11	0.26	0.22
1U59	0.15	0.11	0.26	0.19
3GOP	0.15	0.11	0.26	0.15
3ZFM	0.15	0.11	0.19	0.11
2QOD	0.15	0.11	0.11	0.11
2QOL	0.15	0.11	0.11	0.11
2QOO	0.15	0.11	0.11	0.11
4X3J	0.15	0.07	0.30	0.19
2OZO	0.15	0.07	0.22	0.11
4K2R	0.15	0.07	0.22	0.11
4UX8	0.15	0.04	0.11	0.07
3QGY	0.11	0.11	0.56	0.41

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
4L7S	0.11	0.11	0.56	0.41
1QPC	0.11	0.11	0.22	0.22
1QPD	0.11	0.11	0.22	0.22
3A4O	0.11	0.11	0.22	0.22
3V5L	0.11	0.11	0.22	0.19
4PQN	0.11	0.11	0.22	0.19
1QCF	0.11	0.11	0.15	0.15
2DQ7	0.11	0.11	0.15	0.15
2HK5	0.11	0.11	0.15	0.15
1YOJ	0.11	0.07	0.11	0.11
1YOL	0.11	0.07	0.07	0.04
4C3F	0.07	0.07	0.19	0.15
1AD5	0.07	0.07	0.15	0.15
1AB2	0.07	0.07	0.07	0.07
3K2M	0.07	0.07	0.07	0.07
4EIH	0.07	0.07	0.07	0.07
2ABL	0.07	0.07	-	-
2ECD	0.07	0.07	-	-
3UIU	0.07	0.04	0.44	0.30
2A19	0.07	0.04	0.41	0.26
4BBF	0.07	0.04	0.30	0.19
4GFU	-	-	0.30	0.19
1A1A	-	-	0.30	0.15
1O4R	-	-	0.30	0.15
4F5B	-	-	0.30	0.15
2EC8	-	-	0.26	0.19
4FVQ	-	-	0.26	0.19
4FVR	-	-	0.22	0.19
4C8B	-	-	0.22	0.15
3OJ2	-	-	0.19	0.15
3OJM	-	-	0.19	0.15
4DKD	-	-	0.19	0.15
4BSJ	-	-	0.19	0.11
1SHY	-	-	0.15	0.15
2BUJ	-	-	0.15	0.15
3ULR	-	-	0.15	0.15
4K3J	-	-	0.15	0.15

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
4O3U	-	-	0.15	0.15
4D2W	-	-	0.15	0.11
4KRP	-	-	0.15	0.11
4L0P	-	-	0.15	0.11
1AWO	-	-	0.15	0.07
1H9O	-	-	0.15	0.07
3EG0	-	-	0.15	0.07
3EG1	-	-	0.15	0.07
4J9E	-	-	0.15	0.07
4J9F	-	-	0.15	0.07
4RA0	-	-	0.15	0.07
2C5D	-	-	0.11	0.11
4QT8	-	-	0.11	0.11
1FBV	-	-	0.11	0.07
1IGR	-	-	0.11	0.07
1NUN	-	-	0.11	0.07
1XR0	-	-	0.11	0.07
2AHX	-	-	0.11	0.07
2BBA	-	-	0.11	0.07
2DCR	-	-	0.11	0.07
2DJS	-	-	0.11	0.07
2DTG	-	-	0.11	0.07
2FDB	-	-	0.11	0.07
2MFQ	-	-	0.11	0.07
3HCK	-	-	0.11	0.07
3LOH	-	-	0.11	0.07
3NHN	-	-	0.11	0.07
3NRU	-	-	0.11	0.07
3U2P	-	-	0.11	0.07
3U3F	-	-	0.11	0.07
3W11	-	-	0.11	0.07
3W12	-	-	0.11	0.07
3W13	-	-	0.11	0.07
3W14	-	-	0.11	0.07
4BKY	-	-	0.11	0.07
4HRL	-	-	0.11	0.07
4OGA	-	-	0.11	0.07

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
4R32	-	-	0.11	0.07
4U5W	-	-	0.11	0.07
4UMQ	-	-	0.11	0.07
4UMT	-	-	0.11	0.07
1GQ5	-	-	0.11	0.04
1M6B	-	-	0.11	0.00
3P11	-	-	0.11	0.00
1A81	-	-	0.07	0.07
1CSY	-	-	0.07	0.07
1IJR	-	-	0.07	0.07
1K04	-	-	0.07	0.07
1LCK	-	-	0.07	0.07
1LKK	-	-	0.07	0.07
1NQL	-	-	0.07	0.07
1WA7	-	-	0.07	0.07
1YRK	-	-	0.07	0.07
1YY9	-	-	0.07	0.07
2CR3	-	-	0.07	0.07
2IFG	-	-	0.07	0.07
2LCT	-	-	0.07	0.07
2OQ1	-	-	0.07	0.07
4D8K	-	-	0.07	0.07
4IXP	-	-	0.07	0.07
1B55	-	-	0.07	0.04
1BTK	-	-	0.07	0.04
1BWN	-	-	0.07	0.04
1HCF	-	-	0.07	0.04
1QR1	-	-	0.07	0.04
1QU6	-	-	0.07	0.04
2A91	-	-	0.07	0.04
2WO1	-	-	0.07	0.04
3G5V	-	-	0.07	0.04
3GM3	-	-	0.07	0.04
3PFV	-	-	0.07	0.04
3QS9	-	-	0.07	0.04
3ZNI	-	-	0.07	0.04
4AG4	-	-	0.07	0.04

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
4BK5	-	-	0.07	0.04
4BKF	-	-	0.07	0.04
4KRM	-	-	0.07	0.04
4M4P	-	-	0.07	0.04
4W50	-	-	0.07	0.04
1FLT	-	-	0.07	0.00
2QBX	-	-	0.07	0.00
4FWW	-	-	0.07	0.00
1CF4	-	-	0.04	0.04
1FYR	-	-	0.04	0.04
1MOX	-	-	0.04	0.04
1MW4	-	-	0.04	0.04
1RHF	-	-	0.04	0.04
1RJA	-	-	0.04	0.04
1RY7	-	-	0.04	0.04
1SHC	-	-	0.04	0.04
1X8B	-	-	0.04	0.04
2CBL	-	-	0.04	0.04
2E7H	-	-	0.04	0.04
2E9W	-	-	0.04	0.04
2K9Y	-	-	0.04	0.04
2KGT	-	-	0.04	0.04
2KK1	-	-	0.04	0.04
2L4K	-	-	0.04	0.04
2LUL	-	-	0.04	0.04
2MC1	-	-	0.04	0.04
2UZX	-	-	0.04	0.04
2X1W	-	-	0.04	0.04
2X2U	-	-	0.04	0.04
2Y1N	-	-	0.04	0.04
3BUO	-	-	0.04	0.04
3BUW	-	-	0.04	0.04
3BUX	-	-	0.04	0.04
3C8X	-	-	0.04	0.04
3FL7	-	-	0.04	0.04
3G5Y	-	-	0.04	0.04
3HEI	-	-	0.04	0.04

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
3MBW	-	-	0.04	0.04
3MJG	-	-	0.04	0.04
3MX0	-	-	0.04	0.04
3OB2	-	-	0.04	0.04
3QS7	-	-	0.04	0.04
3QWQ	-	-	0.04	0.04
3S35	-	-	0.04	0.04
3V2A	-	-	0.04	0.04
3ZMP	-	-	0.04	0.04
3ZMQ	-	-	0.04	0.04
4A4B	-	-	0.04	0.04
4A4C	-	-	0.04	0.04
4BSK	-	-	0.04	0.04
4DYL	-	-	0.04	0.04
4EKU	-	-	0.04	0.04
4GS0	-	-	0.04	0.04
4L00	-	-	0.04	0.04
4L01	-	-	0.04	0.04
4LEO	-	-	0.04	0.04
4LIQ	-	-	0.04	0.04
1EVT	-	-	0.04	0.00
1WWC	-	-	0.04	0.00
1WWW	-	-	0.04	0.00
1Z9I	-	-	0.04	0.00
2GY5	-	-	0.04	0.00
2HR7	-	-	0.04	0.00
2K1L	-	-	0.04	0.00
2M20	-	-	0.04	0.00
3H3B	-	-	0.04	0.00
3OJV	-	-	0.04	0.00
3RBB	-	-	0.04	0.00
4HRN	-	-	0.04	0.00
4K0V	-	-	0.04	0.00
4NY0	-	-	0.04	0.00
4PO6	-	-	0.04	0.00
1AOT	-	-	-	-
1AWW	-	-	-	-

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
1B4F	-	-	-	-
1BU1	-	-	-	-
1CSK	-	-	-	-
1EFN	-	-	-	-
1EV2	-	-	-	-
1F62	-	-	-	-
1G83	-	-	-	-
1HE7	-	-	-	-
1II4	-	-	-	-
1MFG	-	-	-	-
1MFL	-	-	-	-
1N8Z	-	-	-	-
1Q68	-	-	-	-
1QLY	-	-	-	-
1SSL	-	-	-	-
1UCV	-	-	-	-
1WWB	-	-	-	-
1X5L	-	-	-	-
1X6G	-	-	-	-
1ZZP	-	-	-	-
2DBJ	-	-	-	-
2DM0	-	-	-	-
2E6I	-	-	-	-
2E8N	-	-	-	-
2EAO	-	-	-	-
2EKX	-	-	-	-
2GE9	-	-	-	-
2HDA	-	-	-	-
2IIM	-	-	-	-
2KK6	-	-	-	-
2KS1	-	-	-	-
2KSO	-	-	-	-
2KUP	-	-	-	-
2KUQ	-	-	-	-
2L6W	-	-	-	-
2L9U	-	-	-	-
2LCX	-	-	-	-

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
2LMJ	-	-	-	-
2LZL	-	-	-	-
2M0B	-	-	-	-
2M59	-	-	-	-
2MET	-	-	-	-
2MEU	-	-	-	-
2MFR	-	-	-	-
2OJ2	-	-	-	-
2QKQ	-	-	-	-
2VIF	-	-	-	-
2WUH	-	-	-	-
2YS2	-	-	-	-
2YS5	-	-	-	-
2YUQ	-	-	-	-
2YUU	-	-	-	-
3BRH	-	-	-	-
3CAF	-	-	-	-
3EAC	-	-	-	-
3EAZ	-	-	-	-
3GRW	-	-	-	-
3H0F	-	-	-	-
3H0H	-	-	-	-
3H8M	-	-	-	-
3HIL	-	-	-	-
3KKA	-	-	-	-
3KVQ	-	-	-	-
3OP0	-	-	-	-
3P0Y	-	-	-	-
3P1I	-	-	-	-
3REA	-	-	-	-
3REB	-	-	-	-
3UA7	-	-	-	-
3US4	-	-	-	-
3V6B	-	-	-	-
3VRO	-	-	-	-
3VRP	-	-	-	-
3VRR	-	-	-	-

Continuation of Table S8

	Mutation settings		Conformation settings	
PDB code	Coverage	Identity	Coverage	Identity
3ZON	-	-	-	-
4CRP	-	-	-	-
4D8D	-	-	-	-
4ET7	-	-	-	-
4HCK	-	-	-	-
4HXJ	-	-	-	-
4J9C	-	-	-	-
4K94	-	-	-	-
4ORZ	-	-	-	-